

Yi Yao, Ph.D.

Resume

Education

- 2012–2018 **PhD in Theoretical/Computational Chemistry**, *Department of Chemistry, The University of North Carolina at Chapel Hill, NC, USA.*
- 2008–2012 **Bachelor of Science with honor in Chemistry**, *Department of Chemical Physics, University of Science and Technology of China, Hefei, China.*

Professional Experience

- 2020- Research Scientist (with Profs. Volker Blum and Yosuke Kanai)
Department of Mechanical Engineering and Materials Science, Duke University
Department of Chemistry, University of North Carolina at Chapel Hill
- 2018-2020 Postdoctoral Researcher (with Profs. Volker Blum and Yosuke Kanai)
Department of Mechanical Engineering and Materials Science, Duke University
Department of Chemistry, University of North Carolina at Chapel Hill
- 2012-2018 Graduate Research Assistant (with Profs. Yosuke Kanai and Max Berkowitz)
Department of Chemistry, University of North Carolina at Chapel Hill
- 2012-2013 Graduate Teaching Assistant
Department of Chemistry, University of North Carolina at Chapel Hill
- 2011-2012 Undergraduate Research Assistant (with Prof. Xiaojun Wu)
Department of Materials Science and Engineering, University of Science and Technology of China

Awards

- Dec. 2020 Best Poster Award, Triangle Hard Matter Workshop
- May. 2017 James T. Dobbins Fellowship, UNC-Chapel Hill
- Oct. 2012 Francis P. Venable Fellowship, UNC-Chapel Hill
- Oct. 2011 Outstanding Student Scholarship (First Grade), USTC, top 3%
- Oct. 2010 Zhang Maosen Scholarship, USTC, top 10%
- Oct. 2009 Outstanding Student Scholarship (Second Grade), USTC, top 10%
- Oct. 2008 Liu Youcheng Scholarship, USTC

Research Expertise

Research Experience	Molecular Dynamics Simulation, First Principles Electronic Structure Theory (Greens Function Theory, Density Functional Theory, Quantum Monte Carlo)
Code Development	QB@LL, FHI/AIMS
Programming Language	C++, PYTHON, FORTRAN

Publications

- [14] All-electron periodic G 0 W 0 implementation with numerical atomic orbital basis functions: Algorithm and benchmarks: *Physical Review Materials* 5 (2021), 1, 013807. Xinguo Ren ; Florian Merz ; Hong Jiang ; **Yi Yao** ; Markus Rampp ; Hermann Lederer ; Volker Blum ; Matthias Scheffler
- [13] Temperature dependence of nuclear quantum effects on liquid water via artificial neural network model based on SCAN meta-GGA functional: *Journal of Chemical Physics* 153 (2020), 4, 044114. **Yi Yao** ; Yosuke Kanai
- [12] All-electron ab initio Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals: *Journal of Chemical Physics* 152 (2020), 4, 044105. Chi Liu ; Jan Kloppenburg ; **Yi Yao** ; Xinguo Ren ; Heiko Appel ; Yosuke Kanai ; Volker Blum
- [11] First-Principles Modeling of Electronic Stopping in Complex Matter Under Ion Irradiation: *Journal of Physical Chemistry Letters* 11 (2020), 1, 229-237. Dillon C Yost ; **Yi Yao** ; Yosuke Kanai
- [10] K-Shell Core-Electron Excitations in Electronic Stopping of Protons in Water from First Principles: *Physical Review Letters* 123 (2019), 6, 066401. **Yi Yao** ; Dillon C Yost ; Yosuke Kanai
- [9] Propagation of maximally localized Wannier functions in real-time TDDFT: *Journal of Chemical Physics* 150 (2019), 19, 194113. Dillon C Yost ; **Yi Yao** ; Yosuke Kanai
- [8] Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and ω B97X-V Exchange-Correlation Functionals: *Journal of Chemical Theory and Computation* 14 (2018), 2, 884-893. **Yi Yao** ; Yosuke Kanai
- [7] Examining real-time time-dependent density functional theory nonequilibrium simulations for the calculation of electronic stopping power: *Physical Review B* 96 (2017), 11, 115134. Dillon C Yost ; **Yi Yao** ; Yosuke Kanai
- [6] Plane-wave pseudopotential implementation and performance of SCAN meta-GGA exchange-correlation functional for extended systems: *Journal of Chemical Physics* 146 (2017), 22, 224105. **Yi Yao** ; Yosuke Kanai

- [5] Electronic stopping power in liquid water for protons and α particles from first principles: *Phys. Rev. B* 94 (2016), Jul, 041108. Kyle G. Reeves ; **Yi Yao** ; Yosuke Kanai
- [4] Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene: *Journal of Chemical Physics* 145 (2016), 12. Kyle G. Reeves*(co-first author) ; **Yi Yao***(co-first author) ; Yosuke Kanai
- [3] Reptation Quantum Monte Carlo calculation of charge transfer: The NaCl dimer: *Chemical Physics Letters* 618 (2015), 236 - 240. **Yi Yao** ; Yosuke Kanai
- [2] Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer: *Journal of Chemical Physics* 143 (2015), 24. **Yi Yao** ; Max L. Berkowitz ; Yosuke Kanai
- [1] Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions: *Journal of Physical Chemistry Letters* 5 (2014), 15, 2711-2716. **Yi Yao** ; Yosuke Kanai ; Max L. Berkowitz

Presentations

- 2020 Invited: Exploitation of symmetry in periodic density functional calculations in FHI-aims code @ FHI-aims Developers' and Users' Meeting 2020
- 2019 K-Shell Core-Electron Excitations in Electronic Stopping of Protons in Water from First Principles @ APS March Meeting 2019
- 2018 Diffusivity of Liquid Water with SCAN Functional accelerated by Neural Network Force Field @ APS March Meeting 2018
- 2017 First-Principles Molecular Dynamics Simulations of NaCl in Water: Performance of Advanced Exchange-Correlation Approximations in Density Functional Theory @ APS March Meeting 2017
- 2016 Role of Inter-molecular Charge Transfer in Simulating Concentration Dependent Water Diffusivity of Aqueous Salt Solutions @ APS March Meeting 2016
- 2016 Phase Transition between Black and Blue Phosphorenes: A Quantum Monte Carlo Study @ APS March Meeting 2016
- 2015 Role of Charge Transfer in Concentration Dependent Water Diffusivity in Ionic Solutions @ The Roger E. Miller Symposium 2015
- 2015 Reptation Quantum Monte Carlo Calculation of Charge Transfer in the Na-Cl Dimer @ APS March Meeting 2015

References

Volker Blum, Associate Professor, Department of Mechanical Engineering and Materials Science, Duke University, vblum@duke.edu, 919-660-5279

Yosuke Kanai, Associate Professor, Department of Chemistry, University of North Carolina at Chapel Hill, ykanai@unc.edu, 919-962-3891

Max Berkowitz, Professor, Department of Chemistry, University of North Carolina at Chapel Hill, maxb@unc.edu, 919-962-1218